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additional databases
NEWS 21 NOV 20 CA/CAplus to MARPAT accession number crossover limit increased
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NEWS 22 DEC 01 CAS REGISTRY updated with new ambiguity codes
NEWS 23 DEC 11 CAS REGISTRY chemical nomenclature enhanced
NEWS 24 DEC 14 WPIDS/WPINDEX/WPIX manual codes updated
NEWS 25 DEC 14 GBFULL and FRFULL enhanced with IPC 8 features and
functionality
NEWS 26 DEC 18 CA/CAplus pre-1967 chemical substance index entries enhanced
with preparation role
NEWS 27 DEC 18 CA/CAplus patent kind codes updated
NEWS 28 DEC 18 MARPAT to CA/CAplus accession number crossover limit increased
to 50,000
NEWS 29 DEC 18 MEDLINE updated in preparation for 2007 reload
NEWS 30 DEC 27 CA/CAplus enhanced with more pre-1907 records

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AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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McIntosh

11/294,932

* * * * * STN Columbus * * * * *

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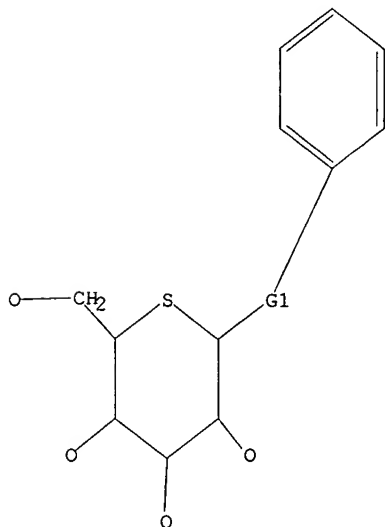
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L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 O,NH

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=> s l1 sss sam

SAMPLE SEARCH INITIATED 12:56:12 FILE 'REGISTRY'

McIntosh

11/294,932

SAMPLE SCREEN SEARCH COMPLETED - 19 TO ITERATE

100.0% PROCESSED 19 ITERATIONS 8 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 119 TO 641
PROJECTED ANSWERS: 8 TO 329

L2 8 SEA SSS SAM L1

=> s l1 full
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FULL SCREEN SEARCH COMPLETED - 412 TO ITERATE

100.0% PROCESSED 412 ITERATIONS 195 ANSWERS
SEARCH TIME: 00.00.01

L3 195 SEA SSS FUL L1

=> file caplus
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FULL ESTIMATED COST 172.10 172.31

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FILE LAST UPDATED: 2 Jan 2007 (20070102/ED)

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<http://www.cas.org/infopolicy.html>

=> s l3
L4 11 L3

=> d bib abs 1-11 14

L4 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:1278776 CAPLUS
TI Preparation of A crystals of 2'-(4'-ethylbenzyl)phenyl
5-thio-β-D-glucopyranoside
IN Sato, Masakazu; Kakinuma, Hiroyuki; Asanuma, Hajime; Amada, Hideaki;
Shinohara, Toshie
PA Taisho Pharmaceutical Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 13pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2006328055	A	20061207	JP 2006-120527	20060425
PRAI	JP 2005-130453	A	20050427		
AB	Title compound (I) having (a) peaks at 2θ = 7.3, 13.2, 19.2, and 21.8° by the powder x-ray diffraction X (Cu-Kα), (b) IR absorption peaks at 1492, 1238, 832, and 742 cm ⁻¹ , and/or (c) DSC exothermic peak at 117-123° and endothermic peak at 157-163°				

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is prepared by (i) dissolving I in organic solvent-water mixture, crystallization at 5-40°, and drying the resulting crystals at 0-65°, or by (ii) suspending I in water (and organic solvent), retaining at 5-30°, and drying the crystals at 0-65°. Thus, I was dissolved in 1:1 EtOH-water mixture at 80°, treated with water, filtered, and dried at 50° in vacuo to give A crystals, which showed good stability at room temperature 75% RH for 4 wk.

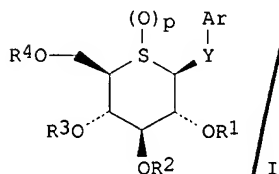
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2006:1278775 CAPLUS
 TI Preparation of C crystals of 2'-(4'-ethylbenzyl)phenyl
 5-thio-β-D-glucopyranoside
 IN Koizumi, Narumi; Shinohara, Toshie
 PA Taisho Pharmaceutical Co., Ltd., Japan
 SO Jpn. Kokai Tokkyo Koho, 12pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2006328054	A	20061207	JP 2006-120515	20060425
PRAI	JP 2005-130454	A	20050427		

AB Title compound (I) having (a) peaks at 2θ = 8.1, 12.8, 19.6, and 23.4° by the powder x-ray diffraction X (Cu-Kα), (b) IR absorption peaks at 1490, 1233, 840, and 745 cm⁻¹, (c) DSC endothermic peak at 157-163°, and/or (d) m.p. 157°-163° is prepared by dissolving I in organic solvent-water mixture, crystallization, and drying the crystals at ≥65°. Thus, I was dissolved in aqueous EtOH, cooled, filtered, and dried at 140° for 3 h to give C crystals, which showed good stability in a sealed container at 40° for 1 mo and higher water solubility than B' crystals.

L4 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2005:1001014 CAPLUS
 DN 143:279419
 TI Inhibitor of sodium-dependent glucose transporter 2
 IN Sato, Masakazu; Kakinuma, Hiroyuki; Asanuma, Hajime
 PA Taisho Pharmaceutical Co., Ltd., Japan
 SO Jpn. Kokai Tokkyo Koho, 70 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2005247834	A	20050915	JP 2005-26180	20050202
PRAI	JP 2004-27413	A	20040204		
OS	MARPAT 143:279419				
GI					



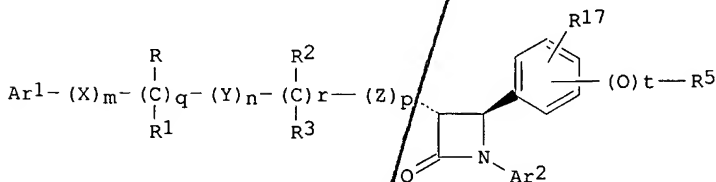
AB The antidiabetic medicines containing 5-thio-β-D-glucopyranoside compound represented by the following general structure I (p = 0 or 1; Y = -O- or -NH-; R1, R2, R3, R4 could be the same or different and = H, C2-10 acyl, C7-10 aralkyl, and C2-6 alkoxy carbonyl etc.) or pharmaceutically acceptable salts as an active component for the inhibition of sodium-dependent glucose transporter 2 (SGLT2) in the kidney are offered. The application of these compds. in the treatment of diabetes mellitus, its complication and its related diseases is discussed.

L4 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2005:423742 CAPLUS
 DN 142:481875

11/294,932

TI Derivatives of 2-azetidinone as antihypercholesterolemic agents
IN Sings, Heather I.; Ujjainwalla, Feroze; Maccoss, Malcolm; Myers, Robert W.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005044256	A1	20050519	WO 2004-US35845	20041027
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	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004286838	A1	20050519	AU 2004-286838	20041027
	CA 2543943	A1	20050519	CA 2004-2543943	20041027
	EP 1682117	A1	20050726	EP 2004-796665	20041027
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
	CN 1870988	A	20061129	CN 2004-80031555	20041027
PRAI	US 2003-515842P	P	20031030		
	WO 2004-US35845	W	20041027		
OS	MARPAT 142:481875				
GI					



AB The present invention provides 2-azetidinone derivs., such as I [Ar¹, Ar² = aryl, R⁴-substituted aryl; X, Y, Z = CH₂, CH(C₁-6alkyl), C(C₁-6alkyl)₂; R = OR₆, OCOR₆, OCO₂R₆, OCONR₆R₇, sugar residue; R₁ = H, alkyl, aryl; R₂ = OR₆, OCOR₆, OCO₂R₆, OCONR₆R₇; R₃ = H, alkyl, aryl; R₂R₃ = oxo; q, r, t = 0 - 1; m, n, p = 0 - 4; R₄ = OR₆, OCOR₆, OCO₂R₉, OCONR₆R₇, COR₆, CONR₆R₇, SO₂NR₆R₇, F; R₅ = R₁₀-R₁₁, R₁₂-R₁₃, OCF₃, NR₆R₇, F; R₆, R₇ = alkyl, aryl, aryl-substituted aryl; R₁₀, R₁₂ = S, SO, SO₂, etc.; R₁₁ = sugar, di-sugar, tri-sugar, tetra-sugar residue; R₁₃ = thiasugar, fluoro-sugar; R₁₇ = H, OH, halo, alkyl, O-alkyl, CF₃, CN, NR₆R₇], and the pharmaceutically acceptable salts and esters thereof, for their use as antihypercholesterolemic agents. The 2-azetidinone derivs. I are useful for lowering plasma cholesterol levels, particularly LDL cholesterol, and for treating and preventing atherosclerosis and atherosclerotic disease events.

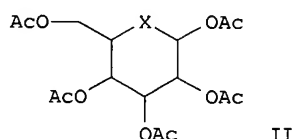
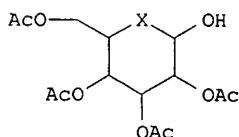
RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:1059367 CAPLUS
DN 142:38476
TI Process for producing aldohexopyranose intermediate
IN Kakinuma, Hiroyuki; Sato, Masakazu; Asanuma, Hajime; Tomisawa, Kazuyuki
PA Taisho Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 22 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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McIntosh

PI WO 2004106352 A1 20041209 WO 2004-JP7556 20040526
 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
 CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
 GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
 LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
 NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
 EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
 SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
 SN, TD, TG
 PRAI JP 2003-151753 A 20030529
 OS CASREACT 142:38476; MARPAT 142:38476
 GI



AB A process for producing a tetra-O-acetylaldohexopyranose represented by the formula (I) (Ac = acetyl; X = O, S; R1 = H, C1-6 alkyl; R2 = C1-6 alkyl, halo-C1-6 alkyl, hydroxy-C1-6 alkyl; or R1 and R2 are bonded to each other and represent, in cooperation with the hydrazine group, optionally substituted N-aminopyrrolidine, N-aminopiperidine, N-aminomorpholine, or N-aminopiperazine, or N-aminoperhydroazepine; R3 = C1-6 alkyl) comprises reacting a penta-O-acetylaldohexopyranose represented by the following formula (II) with a mixture of a hydrazine compound represented by R1R2NNH2 and an organic acid represented by R3COOH to selectively remove an acetyl group at the anomeric position. Thus, to a solution of 42.0 g 1,2,3,4,6-penta-O-acetyl-5-thio-D-glucopyranose in 300 mL DMF was added a mixture of 5.76 g methylhydrazine, 7.50 g AcOH, and 125 mL DMF and the resulting mixture was stirred at room temperature for 2 h, followed by adding an addnl. mixture of 0.967 g methylhydrazine, 1.26 g AcOH, and 21 mL DMF and stirring for addnl. 1 h. The reaction mixture was diluted with 40 mL EtOAc and poured into 400 mL saturated aqueous NaCl, followed by separating the organic layer, successively washing it with 0.5 M aqueous HCl and 400 mL saturated aqueous NaCl, drying over MgSO4, concentration, and purification using silica gel chromatog., 26.5 g 2,3,4,6-tetra-O-acetyl-5-thio-D-glucopyranose (70% yield).

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:872802 CAPLUS

DN 141:366420

TI Method for selective preparation of heteroaryl 5-thio-β-D-aldohexopyranoside by Mitsunobu reaction of heteroaryl alcohols with 5-thio-β-D-aldohexopyranose derivative

IN Kakinuma, Hiroyuki; Sato, Masakazu; Amada, Hideaki; Asanuma, Hajime; Tsuchiya, Yuko

PA Taisho Pharmaceutical Co., Ltd., Japan

SO PCT Int. Appl., 105 pp.

CODEN: PIXXD2

DT Patent

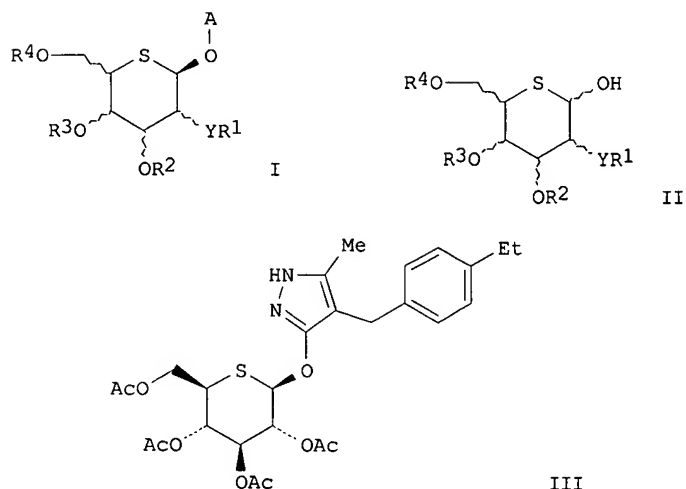
LA Japanese

FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004089966	A1	20041021	WO 2004-JP1244	20040206
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RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,			

11/294,932

ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
 TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 CN 1761676 A 20060419 CN 2004-80007740 20040206
 PRAI JP 2003-97838 A 20030401
 JP 2003-404959 A 20031203
 OS MARPAT 141:366420
 GI



AB Disclosed is a method for preparing a heteroaryl 5-thio-β-D-aldoheptopyranoside compound of the formula (I) [wherein Y = O, NH; R1-R4 = H, C2-10 aryl, C1-6 alkyl, C7-10 aralkyl, C1-6 alkoxy-C7-10 aralkyl, allyl, tri(C1-6 alkyl)silyl, C1-6 alkoxy-C1-6 alkyl, C2-6 alkoxy-carbonyl; or when Y = O, R1 and R2 or R2 and R3 are combined together to form (un)substituted CH2; A = (un)substituted heteroaryl], which comprises reacting 5-thio-D-aldoheptopyranose compound of the formula (II) (wherein R1-R4 = same as above) with heteroaryl alc. of formula A-OH (A = same as above) in the presence of a phosphine represented by PRXRZR [wherein RX, RY, RZ = C1-6 alkyl, (un)substituted Ph, pyridyl, C1-6 alkyl] and an azo reagent represented by R21-N=N-R22 [wherein R21, R22 = C2-5 alkoxy-carbonyl, N,N-di(C1-4 alkyl)aminocarbonyl, piperidinocarbonyl]. Heteroaryl 5-thio-β-D-aldoheptopyranosides are useful as inhibitors of sodium-dependent glucose transporter 2 (SGLT2) (no data). Thus, 5.1 mmol di-Et azodicarboxylate (40% toluene solution) was added dropwise to a solution of 2,3,4,6-tetra-O-acetyl-5-thio-D-glucopyranose (937 mg, 2.6 mmol) and 1,2-dihydro-4-(4-ethylbenzyl)-5-methyl-3H-pyrazol-3-one (2.78 g, 12.9 mmol) and PPh3 (1.35 g, 5.1 mmol) in 14 mL THF at room temperature, stirred for at room temperature for 4 h, and concentrated to give, after silica gel chromatog., 20% β-D-thioglucofuranoside compound (III).

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2004:143171 CAPLUS
 DN 140:199631

TI Preparation of aryl 5-thio-β-D-glucopyranoside derivatives as
 remedies for diabetes

IN Sato, Masakazu; Kakinuma, Hiroyuki; Asanuma, Hajime
 PA Taisho Pharmaceutical Co., Ltd., Japan

SO PCT Int. Appl., 106 pp.
 CODEN: PIXXD2

DT Patent
 LA Japanese

FAN.CNT 2

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PI WO 2004014931	A1	20040219	WO 2003-JP10160	20030808
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PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
 TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
 FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
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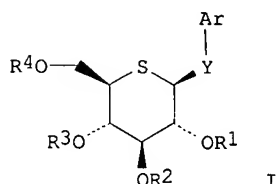
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 AU 2003254904 A1 20040225 AU 2003-254904 20030808
 BR 2003010006 A 20050215 BR 2003-10006 20030808
 EP 1528066 A1 20050504 EP 2003-784623 20030808

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

CN 1639180 A 20050713 CN 2003-805640 20030808
 CN 1675233 A 20050928 CN 2003-819142 20030808
 NZ 535229 A 20060526 NZ 2003-535229 20030808
 JP 3813160 B2 20060823 JP 2004-527383 20030808
 NO 2004003733 A 20041020 NO 2004-3733 20040907
 ZA 2004007187 A 20060222 ZA 2004-7187 20040908
 US 2005209309 A1 20050922 US 2004-518788 20041221

PRAI JP 2002-233015 A 20020809
 JP 2003-97839 A 20030401
 WO 2003-JP10160 W 20030808

OS MARPAT 140:199631
 GI



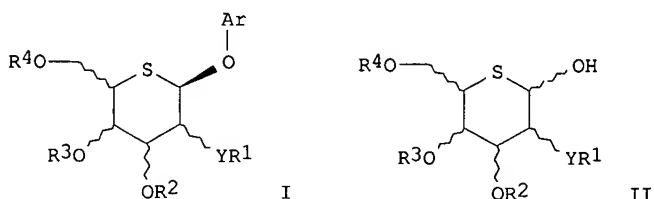
AB The title compds. I [Y = O, etc.; R1 - R4 = H, acyl, etc.; Ar = aryl having substituents (further details on said substituents are given)] are prepared I are inhibitors of SGL T2 (sodium dependent glucose cotransporter 2). In an in vitro test for the inhibition of glucose uptake into brush border membrane vesicles of rat kidney, compds. of this invention showed IC50 values of 0.16 μ M to 2.4 μ M.

RE.CNT 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2004:143170 CAPLUS
 DN 140:199630
 TI Process for selective production of aryl 5-thio- β -D-aldohexopyranosides
 IN Sato, Masakazu; Kakinuma, Hiroyuki; Asanuma, Hajime
 PA Taisho Pharmaceutical Co., Ltd., Japan
 SO PCT Int. Appl., 71 pp.
 CODEN: PIXXD2
 DT Patent
 LA Japanese
 FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004014930	A1	20040219	WO 2003-JP10159	20030808
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2493491	A1	20040219	CA 2003-2493491	20030808
AU 2003254903	A1	20040225	AU 2003-254903	20030808
EP 1541578	A1	20050615	EP 2003-784622	20030808
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1639180	A	20050713	CN 2003-805640	20030808
CN 1675233	A	20050928	CN 2003-819142	20030808
ZA 2004007187	A	20060222	ZA 2004-7187	20040908
US 2005256317	A1	20051117	US 2005-521809	20050121
NO 2005000650	A	20050304	NO 2005-650	20050207
PRAI JP 2002-233015	A	20020809		
JP 2003-97839	A	20030401		
WO 2003-JP10159	W	20030808		
OS MARPAT 140:199630				
GI				

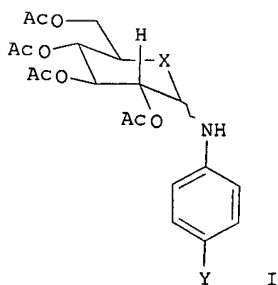


10/5/21/2009
— this is drawn to methods of making my cards.
— allowed
— same priority date

AB This document discloses a process for the production of aryl 5-thio- β -D-aldohecopyranoside derivative I [the wavy line indicates D isomer, L isomer, etc.; Y = O, etc.; R1 - R4 = H, acyl, etc.; Ar = (un)substituted aryl] by reacting a 5-thio-D-aldohecopyranose derivative II [R1 - R4, wavy line = as given above] with ArOH [Ar = as given above] in the presence of a phosphine and an azo reagent.

RE.CNT 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 1999:799909 CAPLUS
 DN 132:208052
 TI Is There a Generalized Reverse Anomeric Effect? Substituent and Solvent Effects on the Configurational Equilibria of Neutral and Protonated N-Arylglucopyranosylamines and N-Aryl-5-thioglucopyranosylamines
 AU Randell, Karla D.; Johnston, Blair D.; Green, David F.; Pinto, B. Mario
 CS Département de Chemistry, Simon Fraser University, Burnaby, BC, V5A 1S6, Can.
 SO Journal of Organic Chemistry (2000), 65(1), 220-226
 CODEN: JOCEAH; ISSN: 0022-3263
 PB American Chemical Society
 DT Journal
 LA English
 GI



AB The effects of substitution and solvent on the configurational equilibrium of neutral and protonated N-(4-Y-substituted-phenyl) peracetylated 5-thioglucopyranosylamines I (X = S; Y = OMe, H, CF3, NO2) (1-4) and N-(4-Y-substituted-phenyl) peracetylated glucopyranosylamines I (X = O; Y = OMe, H, NO2) (9-11) are described. The configurational equilibrium were determined by direct integration of the resonances of the individual isomers in

the ¹H NMR spectra after equilibration of both α - and β -isomers. The equilibrations of the neutral compds. 1-4 in CD₃OD, CD₃NO₂, and (CD₃)₂CO were achieved by HgCl₂ catalysis and those of the neutral compds. 9-11 in CD₂Cl₂ and CD₃OD by triflic acid catalysis. The equilibrations of the protonated compds. in both the sulfur series (solvents, CD₃OD, CD₃NO₂, (CD₃)₂CO, CDCl₃, and CD₂Cl₂) and oxygen series (solvents, CD₂Cl₂ and CD₃OD) were achieved with triflic acid. The substituent and solvent effects on the equilibrium are discussed in terms of steric and electrostatic effects and orbital interactions associated with the endo-anomeric effect. A generalized reverse anomeric effect does not exist in neutral or protonated N-aryl-5-thiogluco-pyranosylamines and N-arylgluco-pyranosylamines. The values of K_{eq}(axial-equatorial) in protonated 1-4 increase in the order OMe < H < CF₃ < NO₂, in agreement with the dominance of steric effects (due to the counterion) over the endo-anomeric effect. The values of K_{eq}(axial-equatorial) in protonated 9-11 show the trend OMe > H < NO₂ that is explained by the balance of the endo-anomeric effect and steric effects in the individual compds.

RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:746389 CAPLUS
DN 132:208047

TI Synthesis and glycosidase inhibitory activity of 5-thiogluco-pyranosylamines. Molecular modeling of complexes with glucoamylase

AU Randell, K. D.; Frandsen, T. P.; Stoffer, B.; Johnson, M. A.; Svensson, B.; Pinto, B. M.

CS Department of Chemistry and Institute of Molecular Biology and Biochemistry, Simon Fraser University, Burnaby, BC, Can.

SO Carbohydrate Research (1999), 321(3-4), 143-156
CODEN: CRBRAT; ISSN: 0008-6215

PB Elsevier Science Ltd.

DT Journal

LA English

AB The synthesis of a series of 5-thio-d-gluco-pyranosylarylamines by reaction of 5-thio-d-gluco-pyranose pentaacetate with the corresponding arylamine and mercuric chloride catalyst is reported. The products were obtained as anomeric mixts. of the tetraacetates which can be separated and crystallized. The tetraacetates were deprotected to give α/β mixts. of the parent compds. which were evaluated as inhibitors of the hydrolysis of maltose by glucoamylase G2 (GA). A transferred NOE NMR experiment with an α/β mixture of p-methoxy-N-phenyl-5-thio-d-gluco-pyranosylamine in the presence of GA showed that only the α isomer is bound by the enzyme. The K_i values, calculated on the basis of specific binding of the α isomers, are 0.47 mM for p-methoxy-N-phenyl-5-thio-d-gluco-pyranosylamine (I), 0.78 mM for N-phenyl-5-thio-d-gluco-pyranosylamine (II), 0.27 mM for p-nitro-N-phenyl-5-thio-d-gluco-pyranosylamine and 0.87 mM for p-trifluoromethyl-N-phenyl-5-thio-d-gluco-pyranosylamine, and the K_m values for the substrates maltose and p-nitrophenyl α -d-gluco-pyranoside are 1.2 and 3.7 mM, resp. Me 4-amino-4-deoxy-4-N-(5'-thio- α -d-gluco-pyranosyl)- α -d-gluco-pyranoside (III) is a competitive inhibitor of GA wild-type (K_i 4 μ M) and the active site mutant Trp120 Phe GA (K_i 0.12 mM). Compds. I-III are also competitive inhibitors of α -glucosidase from brewer's yeast, with K_i 10 mM, and 0.5 mM, resp. Mol. modeling of the inhibitors in the catalytic site of GA was used to probe the ligand-enzyme complementary interactions and to offer insight into the differences in inhibitory potencies of the ligands.

RE.CNT 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1997:319308 CAPLUS
DN 127:17878

TI Relative nucleophilicity of the two sulfur atoms in 1,5-dithiogluco-pyranoside

AU Yuasa, Hideya; Kamata, Yujiro; Hashimoto, Hironobu

CS Faculty Bioscience Biotechnology, Tokyo Inst. Technology, Yokohama, 226, Japan

SO Angewandte Chemie, International Edition in English (1997), 36(8), 868-870
CODEN: ACIEAY; ISSN: 0570-0833

PB VCH

DT Journal

LA English

AB Anomeric effect on the regioselective S-oxidation of thiogluco-pyranoside with

11/294,932

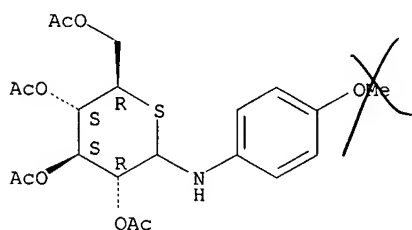
mCPBA is reported.

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d bib hitstr 9-11 14

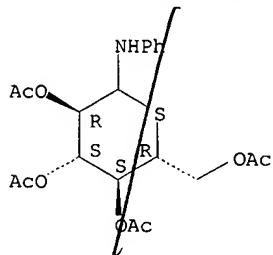
L4 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:799909 CAPLUS
DN 132:208052
TI Is There a Generalized Reverse Anomeric Effect? Substituent and Solvent Effects on the Configurational Equilibria of Neutral and Protonated N-Arylglucopyranosylamines and N-Aryl-5-thiogluco-pyranosylamines
AU Randell, Karla D.; Johnston, Blair D.; Green, David F.; Pinto, B. Mario
CS Department of Chemistry, Simon Fraser University, Burnaby, BC, V5A 1S6, Can.
SO Journal of Organic Chemistry (2000), 65(1), 220-226
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
IT 260793-72-4 260793-73-5 260793-74-6
260793-75-7 260793-76-8 260793-77-9
260793-78-0 260793-80-4 260793-89-3
260793-90-6 260793-91-7 260793-92-8
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(substituent and solvent effects on the configurational equilibrium of neutral and protonated N-arylglucopyranosylamines and N-arylthiogluco-pyranosylamines)
RN 260793-72-4 CAPLUS
CN D-Glucopyranosylamine, N-(4-methoxyphenyl)-5-thio-, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 260793-73-5 CAPLUS
CN D-Glucopyranosylamine, N-phenyl-5-thio-, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

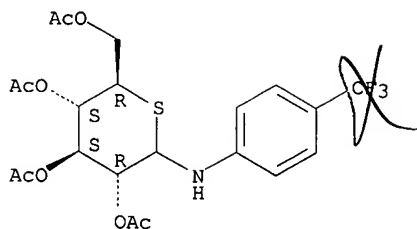


RN 260793-74-6 CAPLUS
CN D-Glucopyranosylamine, 5-thio-N-[4-(trifluoromethyl)phenyl]-, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

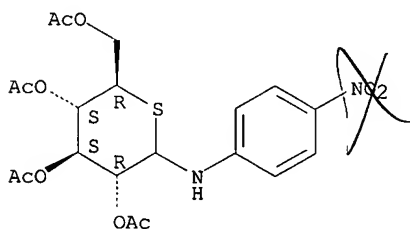
McIntosh

11/294,932



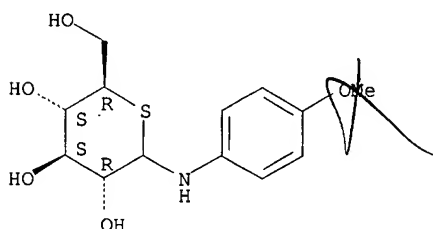
RN 260793-75-7 CAPLUS
CN D-Glucopyranosylamine, N-(4-nitrophenyl)-5-thio-, 2,3,4,6-tetraacetate
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



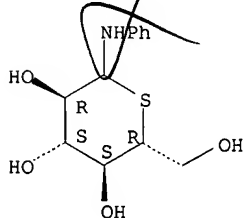
RN 260793-76-8 CAPLUS
CN D-Glucopyranosylamine, N-(4-methoxyphenyl)-5-thio- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 260793-77-9 CAPLUS
CN D-Glucopyranosylamine, N-phenyl-5-thio- (9CI) (CA INDEX NAME)

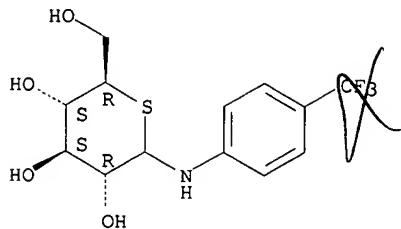
Absolute stereochemistry.



RN 260793-78-0 CAPLUS
CN D-Glucopyranosylamine, 5-thio-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

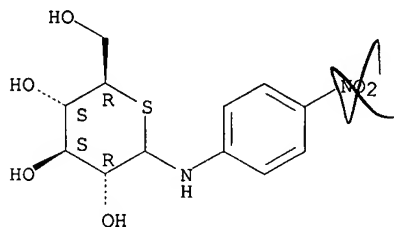
11/294,932



RN 260793-80-4 CAPLUS

CN D-Glucopyranosylamine, N-(4-nitrophenyl)-5-thio- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 260793-89-3 CAPLUS

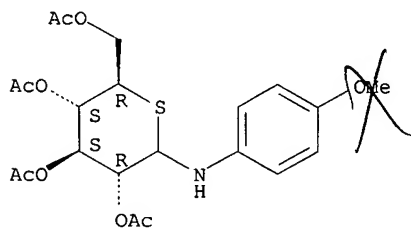
CN D-Glucopyranosylamine, N-(4-methoxyphenyl)-5-thio-, 2,3,4,6-tetraacetate, trifluoromethanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 260793-72-4

CMF C21 H27 N O9 S

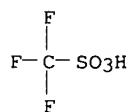
Absolute stereochemistry.



CM 2

CRN 1493-13-6

CMF C H F3 O3 S



RN 260793-90-6 CAPLUS

CN D-Glucopyranosylamine, N-phenyl-5-thio-, 2,3,4,6-tetraacetate, trifluoromethanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

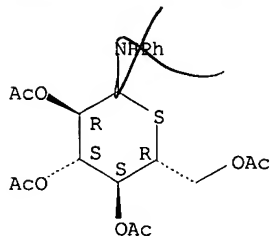
CRN 260793-73-5

CMF C20 H25 N O8 S

McIntosh

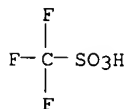
11/294,932

Absolute stereochemistry.



CM 2

CRN 1493-13-6
CMF C H F3 O3 S

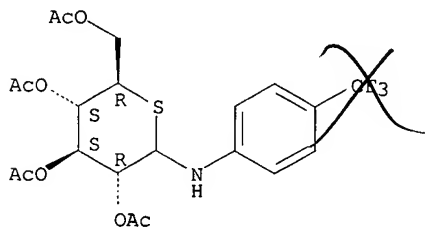


RN 260793-91-7 CAPLUS
CN D-Glucopyranosylamine, 5-thio-N-[4-(trifluoromethyl)phenyl]-,
2,3,4,6-tetraacetate, trifluoromethanesulfonate (salt) (9CI) (CA INDEX
NAME)

CM 1

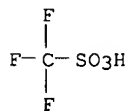
CRN 260793-74-6
CMF C21 H24 F3 N O8 S

Absolute stereochemistry.



CM 2

CRN 1493-13-6
CMF C H F3 O3 S



RN 260793-92-8 CAPLUS
CN D-Glucopyranosylamine, N-(4-nitrophenyl)-5-thio-, 2,3,4,6-tetraacetate,
mono(trifluoromethanesulfonate) (salt) (9CI) (CA INDEX NAME)

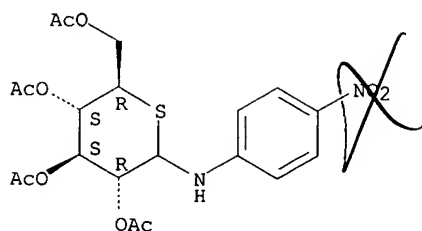
CM 1

CRN 260793-75-7
CMF C20 H24 N2 O10 S

Absolute stereochemistry.

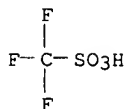
McIntosh

11/294,932



CM 2

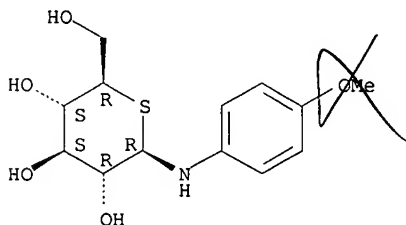
CRN 1493-13-6
CMF C H F3 O3 S



RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:746389 CAPLUS
DN 132:208047
TI Synthesis and glycosidase inhibitory activity of 5-
thioglucopyranosylamines. Molecular modeling of complexes with
glucoamylase
AU Randell, K. D.; Frandsen, T. P.; Stoffer, B.; Johnson, M. A.; Svensson,
B.; Pinto, B. M.
CS Department of Chemistry and Institute of Molecular Biology and
Biochemistry, Simon Fraser University, Burnaby, BC, Can.
SO Carbohydrate Research (1999), 321(3-4), 143-156
CODEN: CRBRAT; ISSN: 0008-6215
PB Elsevier Science Ltd.
DT Journal
LA English
IT 260360-94-9P 260360-95-0P 260360-96-1P
260360-97-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); BIOL (Biological
study); PREP (Preparation)
(synthesis and glycosidase inhibitory activity of
thioglucopyranosylamines. mol. modeling of complexes with glucoamylase)
RN 260360-94-9 CAPLUS
CN β -D-Glucopyranosylamine, N-(4-methoxyphenyl)-5-thio- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.

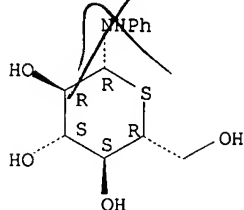


RN 260360-95-0 CAPLUS
CN β -D-Glucopyranosylamine, N-phenyl-5-thio- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

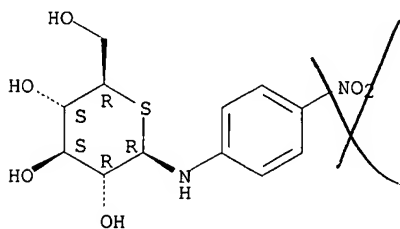
McIntosh

11/294,932



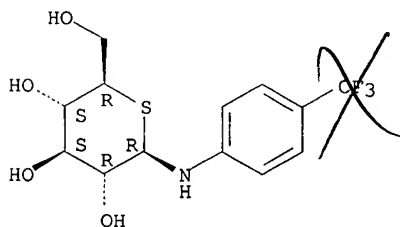
RN 260360-96-1 CAPLUS
CN β -D-Glucopyranosylamine, N-(4-nitrophenyl)-5-thio- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 260360-97-2 CAPLUS
CN β -D-Glucopyranosylamine, 5-thio-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

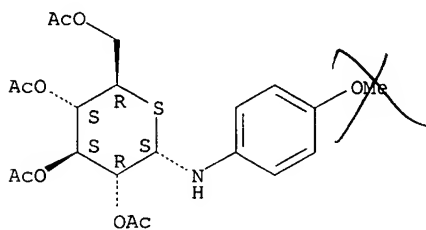
Absolute stereochemistry.



IT 260360-86-9P 260360-87-0P 260360-88-1P
260360-89-2P 260360-90-5P 260360-91-6P
260360-92-7P 260360-93-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and glycosidase inhibitory activity of thioglucopyranosylamines. mol. modeling of complexes with glucoamylase)

RN 260360-86-9 CAPLUS
CN α -D-Glucopyranosylamine, N-(4-methoxyphenyl)-5-thio-, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

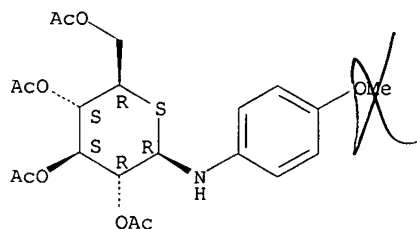


RN 260360-87-0 CAPLUS
CN β -D-Glucopyranosylamine, N-(4-methoxyphenyl)-5-thio-, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

McIntosh

11/294,932

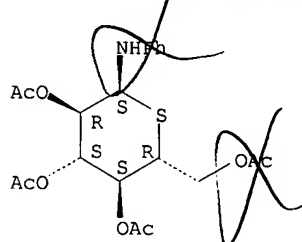
Absolute stereochemistry. Rotation (-).



RN 260360-88-1 CAPLUS

CN α -D-Glucopyranosylamine, N-phenyl-5-thio-, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

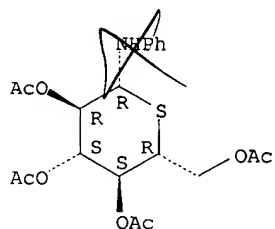
Absolute stereochemistry.



RN 260360-89-2 CAPLUS

CN β -D-Glucopyranosylamine, N-phenyl-5-thio-, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

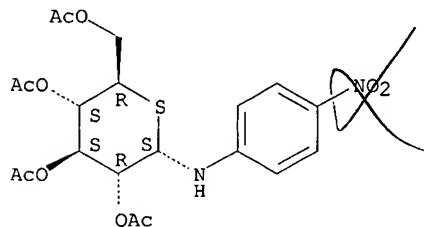
Absolute stereochemistry. Rotation (-).



RN 260360-90-5 CAPLUS

CN α -D-Glucopyranosylamine, N-(4-nitrophenyl)-5-thio-, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



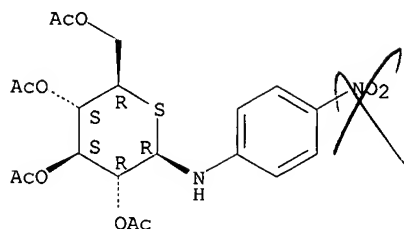
RN 260360-91-6 CAPLUS

CN β -D-Glucopyranosylamine, N-(4-nitrophenyl)-5-thio-, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

McIntosh

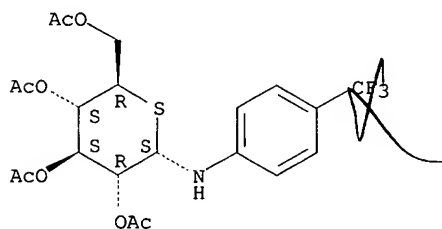
11/294,932



RN 260360-92-7 CAPLUS

CN α -D-Glucopyranosylamine, 5-thio-N-[4-(trifluoromethyl)phenyl]-, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

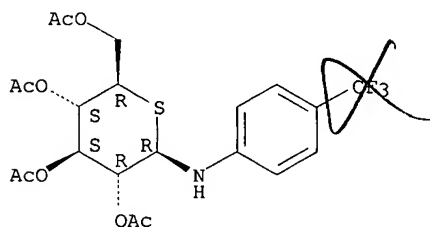
Absolute stereochemistry.



RN 260360-93-8 CAPLUS

CN β -D-Glucopyranosylamine, 5-thio-N-[4-(trifluoromethyl)phenyl]-, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1997:319308 CAPLUS

DN 127:17878

TI Relative nucleophilicity of the two sulfur atoms in 1,5-dithioglucopyranoside

AU Yuasa, Hideya; Kamata, Yujiro; Hashimoto, Hironobu

CS Faculty Bioscience Biotechnology, Tokyo Inst. Technology, Yokohama, 226, Japan

SO Angewandte Chemie, International Edition in English (1997), 36(8), 868-870
CODEN: ACIEAY; ISSN: 0570-0833

PB VCH

DT Journal

LA English

IT 190649-56-0 190649-57-1 190649-58-2

190649-59-3 190649-60-6 190649-61-7

190649-62-8 190649-63-9 190649-64-0

190649-65-1 190649-66-2 190649-67-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(relative nucleophilicity of the two sulfur atoms in
dithioglucopyranoside during regioselective S-oxidation with mCPBA)

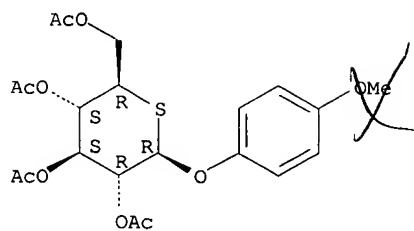
RN 190649-56-0 CAPLUS

CN β -D-Glucopyranoside, 4-methoxyphenyl 5-thio-, tetraacetate (9CI) (CA INDEX NAME)

McIntosh

11/294,932

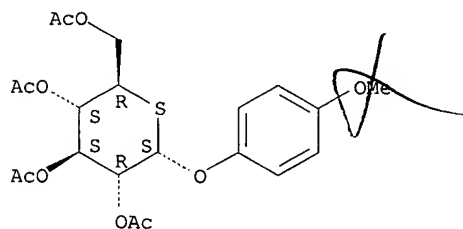
Absolute stereochemistry.



RN 190649-57-1 CAPLUS

CN α -D-Glucopyranoside, 4-methoxyphenyl 5-thio-, tetraacetate (9CI)
(CA INDEX NAME)

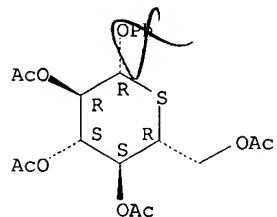
Absolute stereochemistry.



RN 190649-58-2 CAPLUS

CN β -D-Glucopyranoside, phenyl 5-thio-, tetraacetate (9CI) (CA INDEX
NAME)

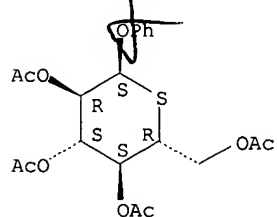
Absolute stereochemistry.



RN 190649-59-3 CAPLUS

CN α -D-Glucopyranoside, phenyl 5-thio-, tetraacetate (9CI) (CA INDEX
NAME)

Absolute stereochemistry.



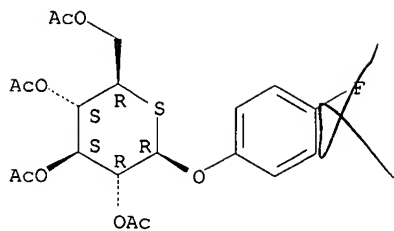
RN 190649-60-6 CAPLUS

CN β -D-Glucopyranoside, 4-fluorophenyl 5-thio-, tetraacetate (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

McIntosh

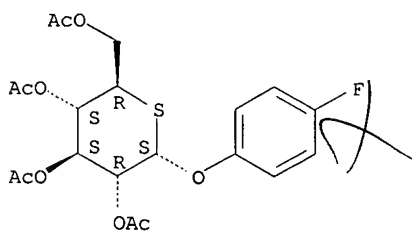
11/294,932



RN 190649-61-7 CAPLUS

CN α -D-Glucopyranoside, 4-fluorophenyl 5-thio-, tetraacetate (9CI) (CA INDEX NAME)

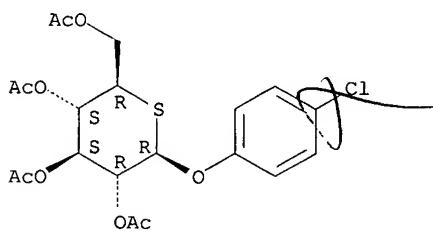
Absolute stereochemistry.



RN 190649-62-8 CAPLUS

CN β -D-Glucopyranoside, 4-chlorophenyl 5-thio-, tetraacetate (9CI) (CA INDEX NAME)

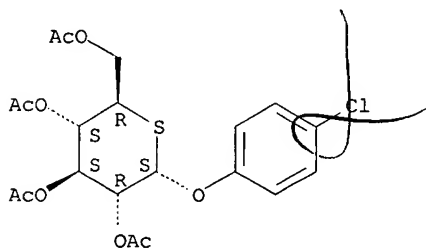
Absolute stereochemistry.



RN 190649-63-9 CAPLUS

CN α -D-Glucopyranoside, 4-chlorophenyl 5-thio-, tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



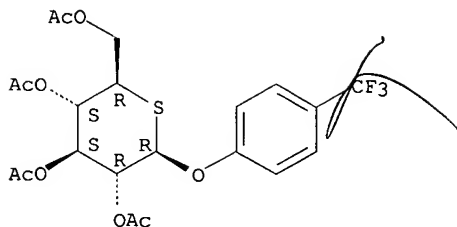
RN 190649-64-0 CAPLUS

CN β -D-Glucopyranoside, 4-(trifluoromethyl)phenyl 5-thio-, tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

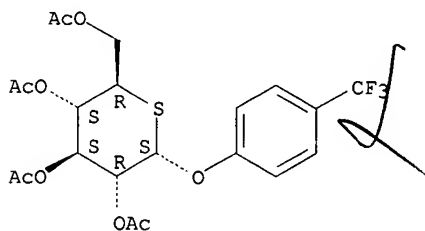
11/294,932



RN 190649-65-1 CAPLUS

CN α -D-Glucopyranoside, 4-(trifluoromethyl)phenyl 5-thio-, tetraacetate
(9CI) (CA INDEX NAME)

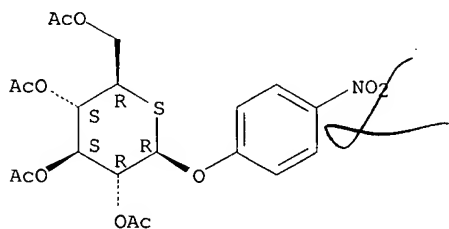
Absolute stereochemistry.



RN 190649-66-2 CAPLUS

CN β -D-Glucopyranoside, 4-nitrophenyl 5-thio-, 2,3,4,6-tetraacetate
(9CI) (CA INDEX NAME)

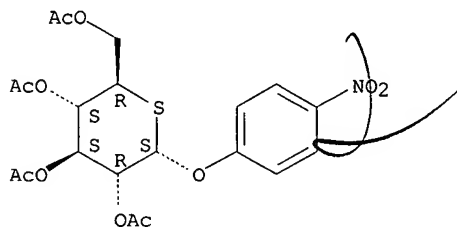
Absolute stereochemistry.



RN 190649-67-3 CAPLUS

CN α -D-Glucopyranoside, 4-nitrophenyl 5-thio-, 2,3,4,6-tetraacetate
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 190649-68-4P 190649-69-5P 190649-70-8P

190649-71-9P 190649-72-0P 190649-73-1P

190649-74-2P 190649-75-3P 190649-76-4P

190649-77-5P 190649-78-6P 190649-79-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(relative nucleophilicity of the two sulfur atoms in
dithioglucopyranoside during regioselective S-oxidation with mCPBA)

RN 190649-68-4 CAPLUS

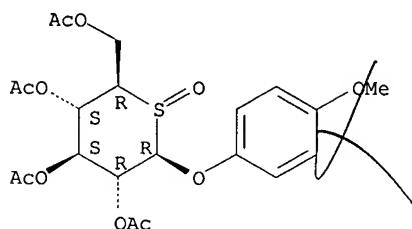
CN β -D-Glucopyranoside, 4-methoxyphenyl 5-thio-, 2,3,4,6-tetraacetate,

McIntosh

11/294,932

S-oxide (9CI) (CA INDEX NAME)

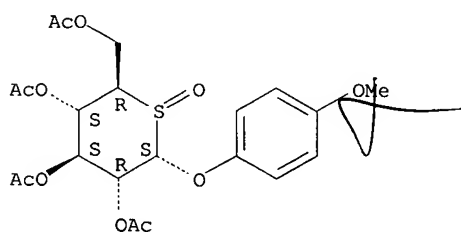
Absolute stereochemistry.



RN 190649-69-5 CAPLUS

CN α -D-Glucopyranoside, 4-methoxyphenyl 5-thio-, 2,3,4,6-tetraacetate, S-oxide (9CI) (CA INDEX NAME)

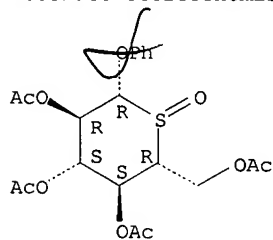
Absolute stereochemistry.



RN 190649-70-8 CAPLUS

CN β -D-Glucopyranoside, phenyl 5-thio-, 2,3,4,6-tetraacetate, S-oxide (9CI) (CA INDEX NAME)

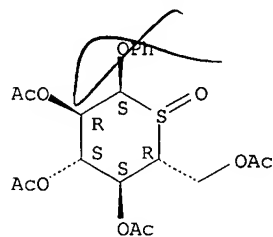
Absolute stereochemistry.



RN 190649-71-9 CAPLUS

CN α -D-Glucopyranoside, phenyl 5-thio-, 2,3,4,6-tetraacetate, S-oxide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



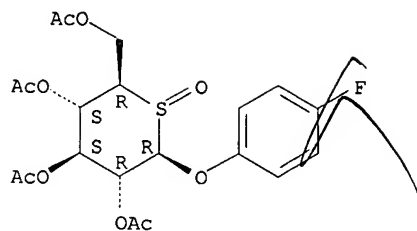
RN 190649-72-0 CAPLUS

CN β -D-Glucopyranoside, 4-fluorophenyl 5-thio-, 2,3,4,6-tetraacetate, S-oxide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

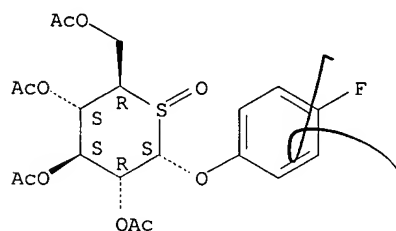
11/294,932



RN 190649-73-1 CAPLUS

CN α -D-Glucopyranoside, 4-fluorophenyl 5-thio-, 2,3,4,6-tetraacetate, S-oxide (9CI) (CA INDEX NAME)

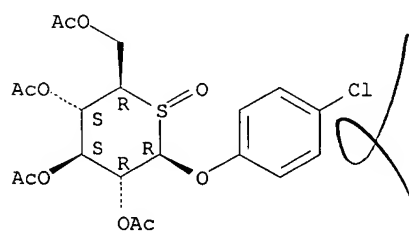
Absolute stereochemistry.



RN 190649-74-2 CAPLUS

CN β -D-Glucopyranoside, 4-chlorophenyl 5-thio-, 2,3,4,6-tetraacetate, S-oxide (9CI) (CA INDEX NAME)

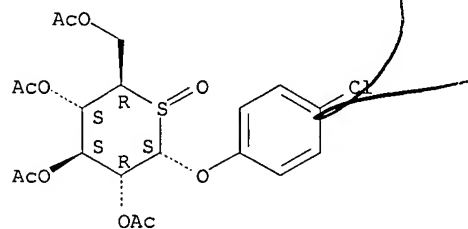
Absolute stereochemistry.



RN 190649-75-3 CAPLUS

CN α -D-Glucopyranoside, 4-chlorophenyl 5-thio-, 2,3,4,6-tetraacetate, S-oxide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



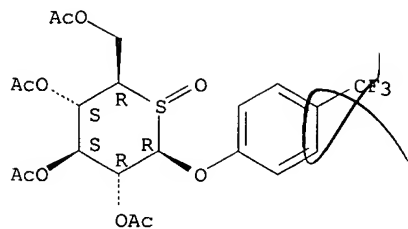
RN 190649-76-4 CAPLUS

CN β -D-Glucopyranoside, 4-(trifluoromethyl)phenyl 5-thio-, 2,3,4,6-tetraacetate, S-oxide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

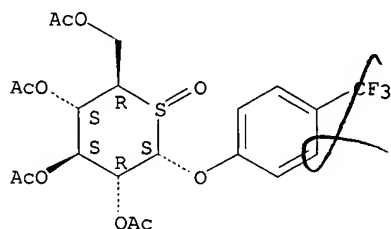
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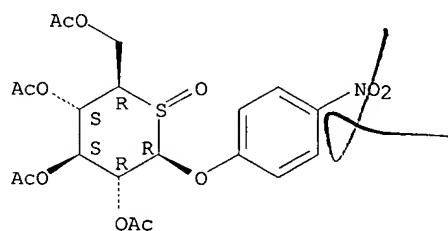
RN 190649-77-5 CAPLUS
CN α -D-Glucopyranoside, 4-(trifluoromethyl)phenyl 5-thio-,
2,3,4,6-tetraacetate, S-oxide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



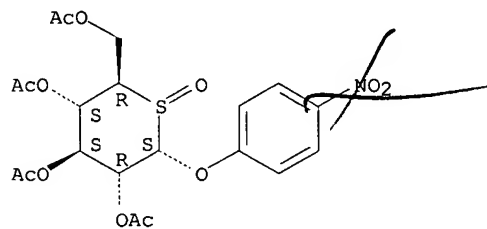
RN 190649-78-6 CAPLUS
CN β -D-Glucopyranoside, 4-nitrophenyl 5-thio-, 2,3,4,6-tetraacetate,
S-oxide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 190649-79-7 CAPLUS
CN α -D-Glucopyranoside, 4-nitrophenyl 5-thio-, 2,3,4,6-tetraacetate,
S-oxide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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